Decoherence and dissipation in quantum two-state systems

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Abstract

The Brownian dynamics of the density operator for a quantum system interacting with a classical heat bath is described using a stochastic, non-linear Liouville equation obtained from a variational principle. The rate of the noise-induced transitions is expressed as a function of the environmental spectral density, and is discussed for the case of white noise and blackbody radiation. The time-scales of decoherence and dissipation are investigated numerically for a system of two quantum states. These are the ground and first excited state of the center of mass vibrations for an ion confined in a harmonic trap.

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I. Introduction

The evolution of a quantum system surrounded by a thermal environment represents a fundamental problem of the quantum theory, increasingly important for applications. In classical mechanics, a particle interacting with a heat bath has a Brownian evolution towards thermalization, which reduces to a purely dissipative motion when the temperature decreases to zero [1]. For a quantum particle, the interaction with the environment is more complex and may produce phenomena without a classical analog, as the collapse of the wave function and decoherence [2]. These effects are particularly important for understanding the mechanism of atom switching in the scanning tunneling microscope [3], for the practical realization of a quantum computer [4] [5], or the transmission of quantum information [6]. However, despite the growing interest in these fields, the physics of the Brownian quantum dynamics and of the wave function decoherence is not yet completely understood [7] [8].

The conceptual difficulties appearing in the description of a quantum system interacting with a classical environment are well illustrated by the

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"Schrödinger cat experiment", or the Zeno paradox at the continuous measurement process [9] [10]. The wave function collapse at macroscopic scale (e.g. of the apparatus pointer) was investigated by Zurek [2], assuming that quantum mechanics describes both the environment and the system. However, when only the system is quantum, the reduction of the density operator by partial tracing over the environment's degrees of freedom is not possible, and the approach should be different. The problem occurs, for instance, in quantum gravity, whenever the space-time framework of a quantum particle remains classical [11]. In such cases, a promising approach to the mixed classical-quantum dynamics consists of using coupled Hamilton-Heisenberg equations derived from a variational principle [12]. The time-dependent variational principle (TDVP) [13] is frequently used in the quantum many-body theory to obtain the mean-field equations (e.g. time-dependent Hartree-Fock). The mean-field dynamics appears by kinematical constraints on the unitary evolution in the many-body Hilbert space, and has a mixed character, including both quantum and classical aspects [14]. Therefore, the TDVP provides an appropriate frame to treat also the mixed version of the bilinear coupling model, consisting of a quantum particle interacting with a heat bath of classical harmonic oscillators. For the pure states, this approach leads to a non-linear time-dependent Schrödinger equation, containing additional noise and friction terms [15]. However, for the treatment of the thermalization process, and evolution from pure to mixed states, it is necessary to include the interaction with the environment in the dynamical equation for the density matrix [16].

In this work, the combined effect produced by noise and dissipation on the quantum evolution will be described using a stochastic, non-linear Liouville equation. This equation can be derived from the variational principle, and will be presented in Sec. II.

The noise represents an external stochastic force which stimulates transitions between the stationary states of the quantum system. A perturbative calculation of the transition rates is presented in Sec. III. The result is compared with the one obtained when the environment is quantized, and is illustrated by two examples: the Gaussian white-noise and the thermal radiation.

The evolution of the density operator when noise and dissipation are both included is investigated numerically in Sec. IV, for the case of a quantum two-state system with relevance for the operation of a logical gate in a quantum computer. This system consists of the ground and first excited state of the center of mass vibrations for a cooled ion in a harmonic trap.

The summary of the results and the conclusions are presented in Sec. V.

II. The stochastic Liouville equation

Let us consider a quantum system with the Hamiltonian and density operators H_0 and ρ, respectively. These operators are Hermitian, and their matrices in an orthonormal basis $\{|e_n\rangle\}$ can be diagonalized by unitary transformations. If $|\Psi_n\rangle(t)$ denotes a normalized eigenstate of $\rho(t)$ corresponding to the eigenvalue w_n, then there exists an unitary operator χ, such that[1] $\rho = \chi D \chi^\dagger$, with $D = \sum_n w_n |e_n\rangle\langle e_n|$. The operator D is related to the von Neumann entropy [17] $S = -Tr(\rho \ln \rho) = -Tr(D \ln D) = -\sum_n w_n \ln w_n$. According to Reznik [18] it is convenient to introduce a "square root operator" η, such that $\rho = \eta\eta^\dagger$. This operator can be defined as $\eta = \chi\sqrt{D}$, and in this case $D = \eta^\dagger\eta = \rho - [\eta, \eta^\dagger]$.

Following the assumptions of the bilinear coupling model [19] [20], a thermal environment can be simulated by a classical heat bath of harmonic oscillators. These will be supposed to be continuously distributed in frequency with the density μ_ω, and interacting with the quantum system by the Hamiltonian $H_{coup} = K \int_0^\infty d\omega \mu_\omega C_\omega q_\omega$. Here K denotes a Hermitian coupling operator, C_ω are constants, and q_ω are the time-dependent bath coordinates. The evolution of this mixed classical-quantum system will be described using the variational equation

$$\delta \int dt \{ \int_0^\infty d\omega \mu_\omega (\dot{q}_\omega p_\omega - h_\omega) + Tr[\eta^\dagger i\hbar \partial_t \eta - \eta^\dagger (H_0 + H_{coup})\eta] \} = 0 \quad , \quad (1)$$

where the dynamical variables of the quantum system are η, $\eta^\dagger$, and $h_\omega = (p_\omega^2 + m_\omega^2 \omega^2 q_\omega^2)/2m_\omega$ is the classical Hamiltonian for a bath oscillator. The equations of motion obtained from Eq. (1) at the variation of $\eta(t)$, $\eta^\dagger(t)$, $q_\omega(t)$ and $p_\omega(t)$ are

$$i\hbar\partial_t \eta = (H_0 + K \int_0^\infty d\omega \mu_\omega C_\omega q_\omega)\eta \ , \ i\hbar\partial_t \eta^\dagger = -\eta^\dagger (H_0 + K \int_0^\infty d\omega \mu_\omega C_\omega q_\omega)$$
$$(2)$$

for the quantum system, and

$$\dot{q}_\omega = \frac{p_\omega}{m_\omega} \ , \ \dot{p}_\omega = -m_\omega \omega^2 q_\omega - C_\omega Tr(K\rho) \qquad (3)$$

for the classical oscillators. The system of Eq. (2) leads to the Liouville equation for the density operator,

$$i\hbar\partial_t \rho = [H_0 + K \int_0^\infty d\omega \mu_\omega C_\omega q_\omega, \rho] \quad . \qquad (4)$$

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[1] In the finite-dimensional case we may consider also the Gauss decomposition $\rho = \chi D \chi^\dagger$ where the matrices χ form a nilpotent group, and D is diagonal.

The classical equations (3) can be solved in terms of the unknown function of time $Q_\rho(t) \equiv Tr(K\rho(t))$, and their retarded solution is

$$q_\omega(t) = [q_\omega(0) + g_\omega Q_\rho(0)] \cos \omega t + \frac{\dot{q}_\omega(0)}{\omega} \sin \omega t$$

$$- g_\omega Q_\rho(t) + g_\omega \int_0^t dt' \dot{Q}_\rho(t') \cos \omega(t - t') \quad , \tag{5}$$

with $g_\omega = C_\omega/(m_\omega \omega^2)$. When this solution is inserted in Eq. (4), the Liouville equation becomes

$$i\hbar \partial_t \rho = [H_0 + W(t), \rho] \tag{6}$$

where $W(t) = -K[\xi(t) + f_\rho(t) + Q_\rho(t)\Gamma(0) - Q_\rho(0)\Gamma(t)]$. The additional term W contains the force functions $\xi(t)$ and $f_\rho(t)$,

$$\xi(t) = -\int_0^\infty d\omega \mu_\omega C_\omega [q_\omega(0) \cos \omega t + \frac{\dot{q}_\omega(0)}{\omega} \sin \omega t] \quad , \tag{7}$$

$$f_\rho(t) = -\int_0^t \Gamma(t - t') \dot{Q}_\rho(t') dt' \quad , \quad \Gamma(t) = \frac{2}{\pi} \int_0^\infty d\omega J(\omega) \frac{\cos \omega t}{\omega} \quad , \tag{8}$$

where $J(\omega) = \pi \omega g_\omega C_\omega \mu_\omega/2$ is the spectral density of the environment. The operator $K[Q_\rho(t)\Gamma(0) - Q_\rho(0)\Gamma(t)]$ ensures the invariance of W to the renormalization of Γ by an additive constant, and vanishes when $\Gamma(t) \sim \delta(t)$ or $Q_\rho(t) = 0$. In the case of a classical heat bath at thermal equilibrium we will assume that Q_ρ and Γ are such that $Q_\rho(t)\Gamma(0) - Q_\rho(0)\Gamma(t) = 0$.

The force function f_ρ makes Eq. (6) non-linear, and therefore, in general, the solutions $\rho(t)$ will not satisfy the superposition principle. Though, exceptions may occur on distinguished "superselection sectors", as the trivial one defined by the set $\{\rho/\dot{Q}_\rho(t) \equiv 0, t \in [0, \infty)\}$.

If the initial coordinates and momenta $q_\omega(0)$, $p_\omega(0)$ are distributed within a statistical ensemble $\mathcal{E}$ with the temperature T, then $\xi(t)$ behaves like a stochastic force which has zero mean and is related to the memory function $\Gamma(t)$ by the fluctuation-dissipation theorem (FDT). Denoting by $\ll * \gg$ the average over $\mathcal{E}$, these properties of ξ are expressed by $\ll \xi(t) \gg = 0$ and $\ll \xi(t)\xi(t') \gg = k_B T \Gamma(t - t')$, respectively. In this case, Eq. (6) becomes a stochastic non-linear Liouville equation for the density operator,

$$i\hbar \partial_t \rho = [H_0 - K(\xi(t) + f_\rho(t)), \rho] \quad . \tag{9}$$

Along the Brownian trajectories $\rho(t)$ obtained by solving this equation, $Tr(\rho^k)$ is a constant for every power $k = 1, 2...$, and therefore the density operator has a Brownian evolution which preserves the "purity" of the

initial state. However, decoherence may appear for the average density operator $\rho_{av}(t) \equiv \ll \rho \gg (t) = \sum_{r=1,N_t} \rho^r(t)/N_t$ calculated over an ensemble of N_t trajectories $\rho^r(t)$ generated with the same initial condition, $\rho^r|_{t=0} = \rho_0$. This average (supposed to be equivalent to the average over $\mathcal{E}$) accounts for the dynamics of the occupation probabilities, and should satisfy a quantum transport equation [2, 20, 21, 22].

III. The noise-induced transitions

When the non-linear friction force f_ρ vanishes or it can be neglected, Eq. (9) becomes

$$i\hbar\partial_t\rho = [H_0 + H_{noise}(t), \rho] \quad, \tag{10}$$

where $H_{noise}(t) = -K\xi(t)$ is the noise term due to the fluctuating environmental forces. This equation has the solution

$$\rho(t) = e^{-iH_0t/\hbar}\tilde{\rho}(t)e^{iH_0t/\hbar} \quad, \quad \tilde{\rho}_{(t)} = \mathcal{T}e^{\frac{i}{\hbar}\int_0^t dt'\xi(t')\mathcal{L}_{\tilde{K}(t')}}\rho_0 \tag{11}$$

where $\mathcal{T}$ denotes the time-ordering operator [23],

$$\tilde{K}(t) = e^{iH_0t/\hbar}Ke^{-iH_0t/\hbar} \tag{12}$$

is the coupling operator in the interaction representation, and $\mathcal{L}_A$ is the Lie derivative with respect to the operator A defined by the commutator, $\mathcal{L}_A B \equiv [A, B]$. The ensemble average of $\rho(t)$ can be written as

$$\rho_{av}(t) = e^{-iH_0t/\hbar}\tilde{\rho}_{av}(t)e^{iH_0t/\hbar} \quad, \tag{13}$$

and the terms appearing in the expansion of the time-ordered exponential defining $\tilde{\rho}_{av}(t)$ can be calculated using the FDT. Retaining only the first non-vanishing average, the result is

$$\tilde{\rho}_{av}(t) = \rho_0 - \frac{k_B T}{\hbar^2}\int_0^t dt_1 \int_0^{t_1} dt_2\Gamma(t_1 - t_2)[\tilde{K}(t_1), [\tilde{K}(t_2), \rho_0]] \quad. \tag{14}$$

This formula can be used to estimate the rate of the noise-induced transitions between the energy eigenstates $\{|E_k\rangle\}$ defined by $H_0|E_k\rangle = E_k|E_k\rangle$. If initially the system is in the pure state $|E_i\rangle$, then $\rho_0 = |E_i\rangle\langle E_i|$, and the rate of the transition $|E_i\rangle \rightarrow |E_f\rangle$ can be defined by the asymptotic time-derivative

$$\lambda_{fi} = \frac{dv_f}{dt}|_{t\rightarrow\infty} \tag{15}$$

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of the occupation probability $v_f(t) = \langle E_f | \rho_{av}(t) | E_f \rangle = \langle E_f | \tilde{\rho}_{av}(t) | E_f \rangle$. Using Eq. (14), this probability is

$$v_f(t) = 2k_B T \frac{|K_{fi}|^2}{\hbar^2} \int_0^t dt_1 \int_0^{t_1} dt_2 \Gamma(t_1 - t_2) \cos[\Omega_{fi}(t_1 - t_2)] \qquad (16)$$

where $K_{fi} = \langle E_f | K | E_i \rangle$ is the matrix element of the coupling operator and $\Omega_{fi} = (E_f - E_i)/\hbar$. The memory function appearing here can be expressed in terms of $J(\omega)$ using Eq. (8), and the transition rate takes the form

$$\lambda_{fi}^{noise} = \frac{2}{\hbar^2} |K_{fi}|^2 k_B T \frac{J(\omega_{fi})}{\omega_{fi}} \quad , \quad \omega_{fi} = |\Omega_{fi}|. \qquad (17)$$

This result was obtained assuming a classical environment, but such cases are rare. Therefore, it is interesting to compare Eq. (17) with the average transition rate λ_{fi}^Q determined by the whole coupling interaction H_{coup} when the bath oscillators are quantized. Let us denote by $|n\rangle$ the eigenstates of Hamiltonian operator $\hat{h}_\omega$ and by $\hat{\rho}_\omega$ the related density operator. At thermal equilibrium, $\hat{\rho}_\omega = Z_\omega^{-1} \exp(-\hat{h}_\omega/k_B T)$ with $Z_\omega = Tr[\exp(-\hat{h}_\omega/k_B T)]$. The correspondent of the trajectory average ρ_{av} is $\rho_{av}^Q(t) \equiv Tr_{\mathcal{E}}[\mathcal{R}(t)]$, defined by the partial trace over the environmental Hilbert space of the density operator $\mathcal{R}$ for the whole system, and within the same approximation as above,

$$v_f(t) = -\frac{1}{\hbar^2} \int_0^t dt_1 \int_0^{t_1} dt_2 \langle E_f | Tr_{\mathcal{E}} \{[\tilde{H}_{coup}(t_1), [\tilde{H}_{coup}(t_2), \mathcal{R}_0]]\} | E_f \rangle . \quad (18)$$

The interaction representation for H_{coup} is defined here with respect to the total Hamiltonian $\mathcal{H}_0 = H_0 + H_{\mathcal{E}}$, $H_{\mathcal{E}} = \int_0^\infty d\omega \mu_\omega \hat{h}_\omega$, and

$$\mathcal{R}_0 = |E_i\rangle \langle E_i| \otimes Z_{\mathcal{E}}^{-1} \exp(-H_{\mathcal{E}}/k_B T) \quad , \qquad (19)$$

with $Z_{\mathcal{E}}$ the partition function of the environment. For an excitation process $|E_i\rangle \rightarrow |E_f\rangle$, Eq. (15) with v_f of Eq. (18) gives the rate

$$\lambda^{\uparrow Q} = \frac{2\pi}{\hbar^2} |K_{fi}|^2 \int_0^\infty d\omega \mu_\omega \sum_{n=1}^\infty (\hat{\rho}_\omega)_{nn} C_\omega^2 |(\hat{q}_\omega)_{n-1,n}|^2 \delta(\omega_{fi} - \omega) \quad , \qquad (20)$$

consisting of the ensemble average of the Fermi's golden rule [24]. This average can be written in the compact form

$$\lambda^{\uparrow Q} = A_{fi} \langle n \rangle_{\omega_{fi}} \quad , \quad A_{fi} = \frac{2}{\hbar} |K_{fi}|^2 J(\omega_{fi}) \quad , \qquad (21)$$

where A_{fi} denotes the rate of the (non-thermal) spontaneous decay, and $\langle n \rangle_\omega = 1/(e^{\hbar\omega/k_B T} - 1)$ is the average number of the bath phonons with energy $\hbar\omega$. Similarly, the total rate for a decay process $|E_f\rangle \to |E_i\rangle$ is $\lambda^{\downarrow Q} = A_{fi}(\langle n \rangle_{\omega_{fi}} + 1) = \lambda^{\uparrow Q} \exp(\hbar\omega_{fi}/k_B T)$. At temperatures $T >> \hbar\omega_{fi}/k_B$ the factor $\langle n \rangle_{\omega_{fi}}$ becomes $\sim k_B T/\hbar\omega_{fi}$, and the rates $\lambda^{\downarrow Q}$, $\lambda^{\uparrow Q}$ practically coincide with λ_{fi}^{noise} of Eq. (17).

According to Eqs. (8) and (17), the friction force and the transition rate are completely determined by the spectral density $J(\omega)$. In the case of Ohmic dissipation $J(\omega) = \gamma\omega$, and the transition rate of Eq. (17) becomes

$$\lambda_{fi}^\Omega = \frac{2}{\hbar^2}|K_{fi}|^2 \gamma k_B T \quad .$$
(22)

The memory function defined by Eq. (8) is singular, reducing to a delta function, $\Gamma(t) = 2\gamma\delta(t)$, and therefore the calculation of the friction force requires a special discussion. For a classical particle with the velocity $\dot{Q}$, the singularity is removed assuming that the cutoff frequency ω_c of μ_ω is such that $\dot{Q}/\omega_c$ is very small, and the delta function is an approximation for a smooth function $\zeta(t)$ [19], peaked at $t = 0$ but non-vanishing for $|t| \neq 0$. The friction force obtained from Eq. (8) using these assumptions is

$$f_\rho(t) = -2\gamma\dot{Q}_\rho(t) \int_0^t \zeta(t - t')dt' = -\gamma\dot{Q}_\rho(t) \quad .$$
(23)

If $\delta(t)$ is supposed to represent the limit of a smooth function defined over the interval $(-\infty, 0]$, then the friction force increases by a factor of 2 with respect to the estimate of Eq. (23), being too strong to ensure thermalization in a classical system. The power dissipated by the friction force of Eq. (23) at $T = 0$, when the noise disappears, is[2]

$$\frac{dE_{diss}}{dt} \equiv -\frac{dTr(H_0\rho)}{dt} = \gamma(\dot{Q}_\rho)^2 = \frac{\gamma}{\hbar^2}|Tr(\rho[H_0, K])|^2 \quad .$$
(24)

Though convenient in calculations, the linear dependence of $J(\omega)$ on ω over the whole spectrum is unrealistic, and it is useful to study also a physical situation of interest. Among the various bilinear coupling systems [25], particularly important is the case of a charged particle interacting with the electromagnetic field. Decoherence produced by spontaneous emission of photons from cold two-level atoms during tunneling through a laser-induced potential barrier was analysed in [26], while a quasiclassical treatment of

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[2]For comparison, the power dissipated in the quantized environment, by a spontaneous decay $|E_f\rangle \to |E_i\rangle$, is $A_{fi}(E_f - E_i) = 2\gamma|\langle E_f|[H_0, K]|E_i\rangle|^2/\hbar^2$.

the bremsstrahlung spectrum for a tunneling charge is presented in [27]. Let us consider here the case of a quantum charged particle interacting with the blackbody radiation field. In the dipolar approximation, the interaction Hamiltonian has the form $H^{rad}_{noise} = -\vec{d} \cdot \vec{E} = -d_x E_x - d_y E_y - d_z E_z$ where $\vec{d} = e\vec{r}$ is the electric dipole operator of the particle, and $\vec{E}$ is the radiation electric field. For isotropic radiation $e\vec{E}$ represents a stochastic force with 0 mean, such that H^{rad}_{noise} is a sum of three terms, each of the form $-K\xi$ assumed above. If the components of the stochastic force are uncorrelated, the FDT is expressed by $e^2 \ll E_i(t)E_j(t') \gg = \delta_{ij}k_B T\Gamma(t - t')$. For $t = t'$, the left-hand side of this equality can be related to the total spectral energy density u_ω,

$$\ll E_i^2(t) \gg = \frac{4\pi}{3}\int_0^\infty d\omega u_\omega \quad , \tag{25}$$

and if $\Gamma(t)$ in the FDT has the form assumed in Eq. (8), then

$$J(\omega) = \frac{2\pi^2 e^2}{3k_B T}\omega u_\omega \quad . \tag{26}$$

For u_ω the realistic expression $u_\omega = \hbar\omega^3\langle n\rangle_\omega/\pi^2 c^3$ can be considered, which accounts for the effects of the second quantization of the radiation field. In this case, the transition rate provided by Eq. (17) is

$$\lambda^{rad}_{fi} = A_{fi}\langle n\rangle_{\omega_{fi}} \tag{27}$$

where

$$A_{fi} = \frac{4e^2}{3\hbar c^3}|\vec{r}_{fi}|^2\omega_{fi}^3 \tag{28}$$

denotes the Einstein coefficient for spontaneous emission. Therefore, λ^{rad}_{fi} is the usual rate of the stimulated transitions in thermal radiation field [28]. The memory function vanishes when $T = 0$, but at high temperatures it becomes proportional to the second derivative of the delta function, $\Gamma(t) = -4e^2\ddot{\delta}(t)/(3c^3)$, and the corresponding friction force

$$\vec{f}_{rad} = \frac{2e^2}{3c^3}\frac{d^3\langle\vec{r}\rangle}{dt^3}, \tag{29}$$

is the classical radiation reaction [29].

IV. Numerical results for a quantum two-state system

The model of a quantum two-state system (TSS) interacting with the environment appears in many physical situations [30]. Usually it is associated

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with the relaxation of a 1/2 spin system, but it was adapted also to study the environmental effects on the quantum coherence oscillations (QCO) in one-dimensional double-well potentials.

A quantum TSS can store one bit of information (qubit), and represents the main component in the design of a quantum computer. The influence of the environment is crucial in this case, because an accurate execution of the logical operations [31] requires a conditional, but unitary evolution of the qubit states. According to Cirac and Zoller, [32] a first generation of quantum logic circuits could be created using cold ions confined in a linear trap. The qubits are reprezented by two-level systems of internal electronic states, while the conditional dynamics required by the logical operations is implemented by their entanglement using the collective states of the center of mass (CM) vibrations. Therefore, the operation time of such computing devices is limited essentially by the occurrence of spontaneous transitions between the electronic states, and the environmental decoherence of the CM vibrational dynamics [33].

The present numerical estimates concern the quantum TSS consisting of the ground ($|0\rangle$) and the first excited state ($|1\rangle$), for the CM vibrations of a single ion trapped in a one dimensional harmonic oscillator potential. Within this restricted two-state Hilbert space, the unperturbed Hamiltonian and the coupling operator can be expressed in terms of the Pauli spin matrices $\sigma_x = |1\rangle\langle1| - |0\rangle\langle0|$, $\sigma_y = |1\rangle\langle0| + |0\rangle\langle1|$, $\sigma_z = i(|0\rangle\langle1| - |1\rangle\langle0|)$. This representation is chosen such that $H_0 = \Delta\sigma_x/2$, and $K = Q\sigma_z$, simulating a coupling linear in the CM coordinate or momentum. For simplicity, the spectrum of the environmental noise will be considered flat (white noise), having the density $J(\omega) = \gamma\omega$. In this case Eq. (9) becomes

$$i\hbar\partial_t\rho = [H_0 - Q\mathcal{F}(t)\sigma_z, \rho] \quad , \tag{30}$$

with $\mathcal{F}(t) = \xi(t) - \gamma\Delta QP_y/\hbar$. Denoting by $\vec{P} \equiv \{P_x, P_y, P_z\}$ the polarization vector, the density operator can be written as $\rho = (I + \vec{P}\cdot\vec{\sigma})/2$ and Eq. (30) takes the explicit form

$$
\begin{aligned}
\hbar\dot{P}_x &= 2Q\mathcal{F}(t)P_y \\
\hbar\dot{P}_y &= -\Delta P_z - 2Q\mathcal{F}(t)P_x \\
\hbar\dot{P}_z &= \Delta P_y
\end{aligned}
\tag{31}
$$

It can be easily seen that $\vec{P}\cdot\vec{P}$ is a constant of motion, and along each trajectory $\vec{P}(t)$ the purity of the states is preserved. However, the evolution from pure to mixed states may appear for $\rho_{av} = \ll \rho \gg \equiv (I + \ll \vec{P} \gg \cdot\vec{\sigma})/2$

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and is described by the dynamics of the average polarization vector $\ll \vec{P} \gg$. The eigenvalues w_0, w_1 of $\ll \rho \gg$ are related to $\ll \vec{P} \gg$ by

$$w_0 = \frac{1 + | \ll \vec{P} \gg |}{2} \quad , \quad w_1 = \frac{1 - | \ll \vec{P} \gg |}{2} \tag{32}$$

and determine the entropy

$$S = -(w_0 \ln w_0 + w_1 \ln w_1) \quad . \tag{33}$$

In the numerical calculations $\Delta = \hbar\omega = 19.74 \ 10^{-9}$ eV was considered, corresponding to a trap frequency $\omega = 30$ MHz [34]. The environmental decoherence of the CM wave functions in a Cirac-Zoller logical gate is due to the heating of the ion vibrational motion, or to the random phase fluctuations of the laser fields [33]. To simulate the global effect of these external factors an effective coupling parameter [30] $\alpha \equiv \gamma Q^2/\hbar = 10^{-4}$ was chosen. This value is somehow large, because it corresponds to a spontaneous decay rate (Eq. (21)), $A_{fi} = 2\alpha\omega = 6$ kHz, greater than the values of practical interest [33]. However, it is small enough to be relevant for understanding the behavior of the system at weak damping. Further decrease of α is not expected to bring new qualitative features, though the numerical calculations may become difficult by the increase of the computer time. The temperature was fixed at $T = 1$ mK, when the thermal energy $k_B T = 86.2 \ 10^{-9}$ eV is relatively high compared to Δ, and the corrections due to the quantization of the environment's degrees of freedom may be considered small. The choice of a high temperature makes the two-state approximation too restrictive for a complete description of the vibrational dynamics, but despite this aspect, it remains suggestive because a linear coupling in the CM coordinate or momentum produces transitions only between consecutive levels.

The numerical integration of Eq. (31) was performed using the D02BAF routine of the NAG library [35] using a time step $dt = 0.658$ ns. The initial condition $\vec{P}(t = 0) = \vec{P}_0$ was chosen to represent a pure state, and the average of the density operator was calculated over an ensemble of $N_t = 1000$ trajectories. For each trajectory the noise $\xi(t)$ at the moment $t_n = ndt$ was expressed by $\xi(t_n) = R_n \sqrt{2k_B T\gamma/dt}$ where $\{R_n, \ n = 1, 2, 3, ...\}$ is a sequence of Gaussian pseudo-random numbers with 0 mean and variance 1. This choice ensures the FDT in discrete form, $\ll \xi(t_j)\xi(t_k) \gg = 2k_B T\gamma\delta_{t_j t_k}/dt$.

The vector $\vec{P}_0$ was taken of the form $\vec{P}_0 = (\cos\Phi, 0, \sin\Phi)$ with $\Phi = 0$ and $\pi/2$. These values of Φ correspond to an initial preparation of the system in the upper stationary state $|1\rangle$, and in the non-stationary linear superposition $(|1\rangle + i|0\rangle)/\sqrt{2}$, respectively.
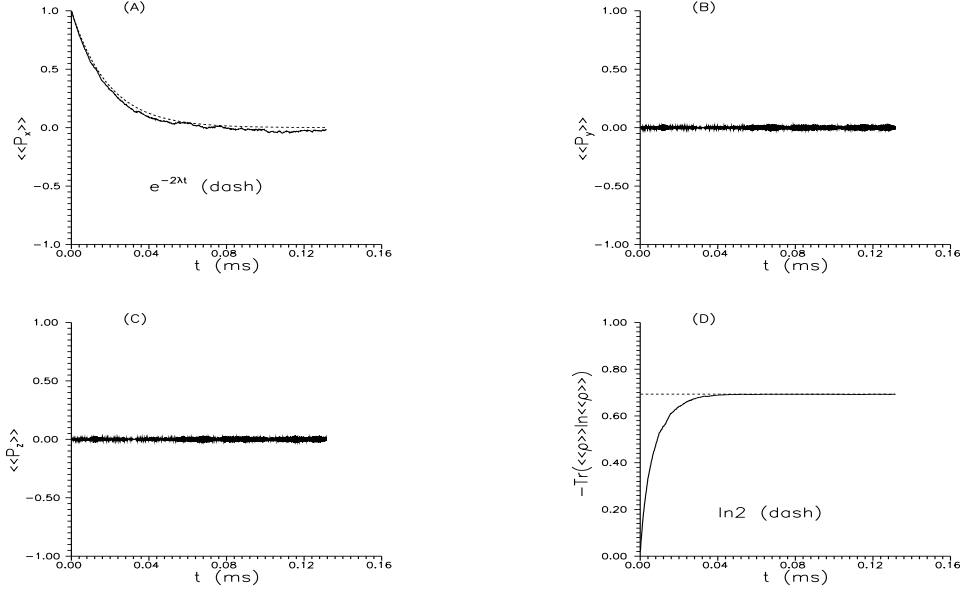
Fig. 1. Ensemble average of the polarization vector (A)-(C), and the entropy (D), as a function of time. The initial condition $\vec{P}_0 = (1, 0, 0)$ corresponds to the upper stationary state $|1\rangle$.

The evolution of the average polarization vector and entropy obtained when $\Phi = 0$ are presented in Fig. 1. The average $\ll P_x \gg$ (Fig. 1 (A), solid line) is very close to the exponential $\exp(-2\lambda t)$ (Fig. 1 (A), dashed line) with $\lambda = 2\alpha k_B T/\hbar = 26.2$ kHz given by Eq. (22). This result is natural, because if the the occupation probabilities $v_0 = \langle 0|\rho_{av}|0\rangle$ and $v_1 = \langle 1|\rho_{av}|1\rangle$ depend on time according to the "phenomenological" rate equations

$$\dot{v}_0 = \lambda^\downarrow v_1 - \lambda^\uparrow v_0 \quad , \quad \dot{v}_1 = -\lambda^\downarrow v_1 + \lambda^\uparrow v_0 \tag{34}$$

then when $\lambda^\uparrow \approx \lambda^\downarrow \approx \lambda$, the relaxation rate of $\ll P_x \gg = v_1 - v_0$ is 2λ. The same rate characterizes the decrease of the energy $E = Tr(\rho_{av} H_0) = \Delta \ll P_x \gg /2$.

The averages $\ll P_y \gg$, $\ll P_z \gg$ presented in Fig. 1 (B),(C), fluctuate around zero, and the main contribution to the variation of the entropy (Fig. 1 (D), solid line) is due to $\ll P_x \gg$. The final value of S is very close to $\ln 2$, (Fig. 1(D), dashed line), the result expected when there is complete decoherence and $w_0 = w_1 = 1/2$. Therefore, the pure state $|1\rangle$ evolves to an incoherent mixture of the two states, $|0\rangle$ and $|1\rangle$. It is interesting to note that the dissipative friction force has a relatively small contribution to the energy decrease. This aspect becomes more clear when $\Phi = \pi/2$. In this case,
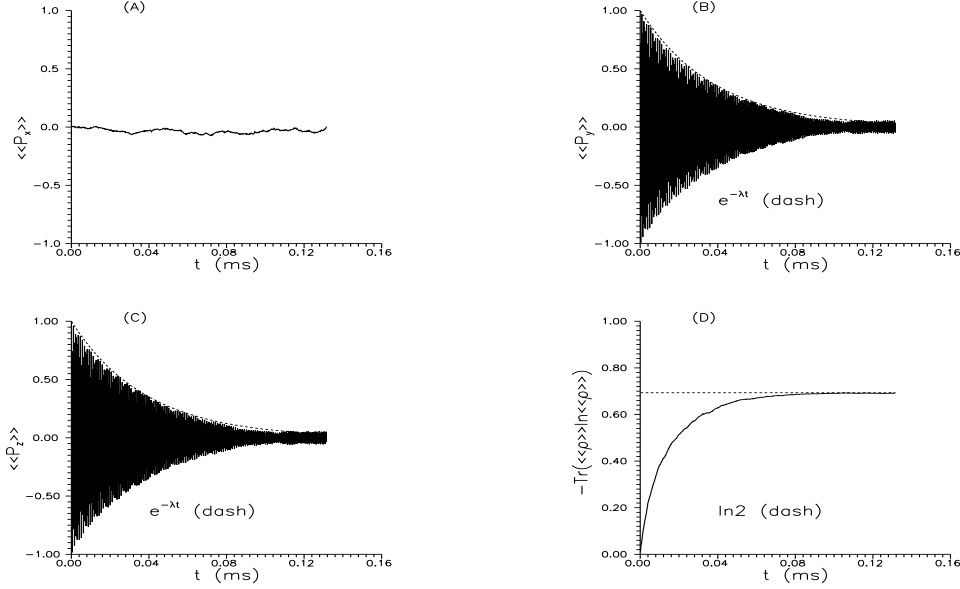
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Fig. 2. Ensemble average of the polarization vector (A)-(C), and the entropy (D), as a function of time. The initial condition $\vec{P}_0 = (0, 0, 1)$ corresponds to the non-stationary superposition $(|1\rangle + i|0\rangle)/\sqrt{2}$.

without environment coupling ($\gamma = 0$), P_x is a constant, while $P_{y,z}$ perform "QCO", $P_y(t) = \sin \omega t$, $P_z(t) = \cos \omega t$. With coupling, the evolution of the average polarization vector and of the entropy are presented in Fig. 2. The average $\ll P_x \gg$ (Fig. 2 (A)) has small fluctuations near the initial value, while the oscillation amplitudes of $\ll P_y \gg$ and $\ll P_z \gg$ decrease exponentially in time[3] (Fig. 2 (B), (C), dashed line) and asymptotically the coherence is lost (Fig. 2 (D)).

In the calculations presented above the average excitation energy $E_x = \Delta/2 + Tr(\rho_{av}H_0)$ changes in time due to the combined effect of noise and friction. When $T > 0$ a well-defined separation between these two contributions is not possible due to the non-linearity, but a measure of the energy which is dissipated by the friction force alone is the ensemble average of E_{diss} from Eq. (24). For the TSS considered above this average has the form $\ll E_{diss} \gg = 0.5\Delta \ll P_x^d \gg$, where $\ll P_x^d \gg$ is the ensemble average

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[3]due to the noise, because for a non-stationary initial state Eq. (14) yields a transport equation, in our case with the solution $\ll P_z \gg + i \ll P_y \gg = e^{-\lambda t} e^{i\Omega t}$, $\Omega = \sqrt{\omega^2 - \lambda^2}$.
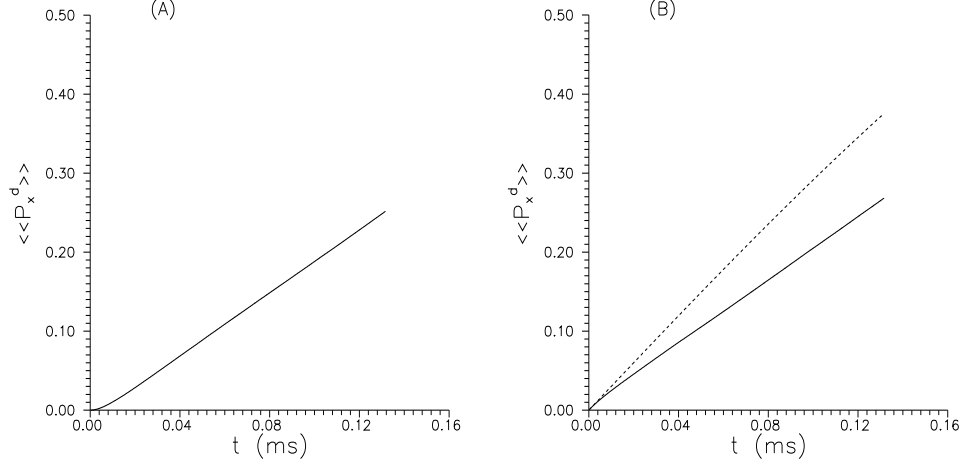
Fig. 3. The ensemble average $\ll P_x^d \gg$ as a function of time when $\vec{P}_0 = (1, 0, 0)$ (A) and $\vec{P}_0 = (0, 0, 1)$ (B, solid line). The short-time behavior of P_x^d calculated without noise (B, dashed line).

of the component P_x^d obtained by integrating the equation

$$\frac{dP_x^d}{dt} = \kappa(t) \quad , \quad \kappa = \frac{2\gamma}{\Delta}(\dot{Q}_\rho)^2 = A_{fi}P_y^2 \quad . \tag{35}$$

The averages $\ll P_x^d \gg$ corresponding to the trajectories presented in Fig. 1 and 2 are pictured in Fig. 3 (A) and (B), respectively, by solid line. After a short transitory time, $\ll \kappa \gg$ becomes practically a constant $\kappa_e \sim 2$ kHz, independently of the initial condition. This constant may provide a measure of the effective coupling between the quantum system and the thermal environment, because at equilibrium the average energy dissipated by friction should be equal to the average energy which is transferred to the system by the thermal noise.

The short time behavior of $\ll P_x^d \gg$ is determined by the frictional forces and the initial state. If $\Phi = \pi/2$ and Eqs. (31) are integrated considering $\xi(t) = 0$, then for small times P_x^d increases linearly in time (Fig. 3 (B), dashed line), with a slope $\kappa_0 = A_{fi}/2 = 3$ kHz. Asymptotically this linear dependence changes to exponential. The numerical calculations show that for $t > t_s \sim 0.4$ ms, $P_x^d(t) \approx \mathcal{P}_s^1(t)$, $\mathcal{P}_s^n(t) = n - [n - P_x^d(t_s)] \exp[-A_{fi}(t - t_s)]$, and the QCO oscillation amplitude is $a_{QCO}(t) \sim a_{QCO}(t_s) \exp[-A_{fi}(t - t_s)/2]$.

When $\Phi = 0$ the friction force vanishes, and without noise ($\xi(t) = 0$), the system remains in the upper stationary state, without dissipation. However,

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if Φ is very small, but not 0, then a_{QCO} increases, attains the maximum, and then decreases, such that after a transitory time t_s, P_x^d has the exponential behavior noticed above, $P_x^d(t) \approx \mathcal{P}_s^2(t)$.

V. Summary and Conclusions

A quantum system in interaction with the surrounding environment has a complex dynamics, which cannot be described only by linear unitary transformations in the Hilbert space between pure states. When the environment is classical, the dynamical equations can be obtained using a time-dependent variational principle. In this work the environment's degrees of freedom have been simulated by classical harmonic oscillators, while the dynamical variables of the quantum system are two non-hermitian "square root operators" η, $\eta^\dagger$, defined by a Gauss-like decomposition of the density matrix.

If the coupling is bilinear, the evolution of the density operator is described by a Liouville equation (Eq. (6)) with an effective Hamiltonian containing two additional terms. One of these terms ($\sim \xi$) is due to the external forces, while the other ($\sim f_\rho$) to the retarded backreaction of the environment on the quantum system, and is non-linear. Therefore, the backreaction term preserves the purity of the states, but may restrict the validity of the superposition principle.

When the environmental oscillators are distributed within a statistical ensemble, the two additional force terms correspond to the noise and friction, being related by the fluctuation-dissipation theorem. In this case, the density operator has a Brownian trajectory corresponding to the evolution from pure to mixed states, described by the ensemble average.

The ensemble average involved in the evaluation of the transition rate between eigenstates can be obtained analytically (Eq. (17)) if the noise is treated as a perturbation and the friction is neglected. For comparison, this average was calculated also when the environment is described by the quantum, rather than classical statistical mechanics, using the partial tracing in the whole Hilbert space (Eq. (21)). As expected, the two averages become close when the thermal energy is greater than the transition energy.

The perturbative transition rates and the frictional forces are given explicitly for an Ohmic environment and for the physical situation of the black-body radiation surrounding a quantum charged particle. This latter example shows that, by a suitable choice of the environmental spectral density, it is possible to recover the stimulated transitions rate provided by the Fermi's golden rule.

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A non-perturbative solution of the stochastic non-linear Liouville equation was obtained numerically for the case of a two-state system coupled to an Ohmic environment. The two states correspond to the ground and first excited state of the CM vibrations for an ion confined in a harmonic trap, at a temperature of 1 mK. Two different initial conditions have been considered, one corresponding to the upper eigenstate of H_0, ($\Phi = 0$), and the other to an eigenstate of the "coordinate" operator K, ($\Phi = \pi/2$). The upper energy eigenstate is also a linear superposition between the two "localized" eigenstates of K, separated by $\Delta_K = 2Q$. For this state, complete decoherence appears when the excitation energy becomes half of the initial value (Fig. 1), after a time $\sim \tau_D = (2\lambda)^{-1} = \hbar^2/(\gamma k_B T \Delta_K^2)$, in agreement with the previous estimates [2]. The decoherence time of the "localized" non-stationary superposition is greater by a factor of 2, but the excitation energy in this case fluctuates near its initial value (Fig. 2).

At high temperatures the power dissipated by friction is relatively small (Fig. 3), with an equilibrium value which is practically independent of the initial state. Without noise, the classical environment produces dissipation only if the initial state is non-stationary (e.g. $\Phi > 0$). For asymptotic times this frictional dissipation resembles closely the spontaneous decay obtained when the environment is quantized.

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